Proceedings of the Fourth International Conference on Tracers and Tracing Applications

Autrans, Grenoble, France, October 3 to 5

Session 8: Environment-Waters and sediments

“A mathematical model for the design and interpretation of tracer experiments intended to measure the T_{90} in estuarine coastal waters”

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Abstract:

In highly stratified estuarine waters, with significant sediment loads, it is fairly difficult to predict the T_{90}, the time scale that characterizes the bacterial inactivation or death, using mathematical formulae, so that suitable experiments must be done using tracers to measure physical dilution and microbiological methods to measure bacterial disappearance or inactivation. The location and characteristics of a second sewage outfall for the city of Montevideo is being determined. In this framework, several experiments with tracers were done to measure the self-purifying capacity of the coastal waters at the selected site. Due to the difficulties in the design and interpretation of the measurements, special mathematical models were constructed and applied to help in obtaining a deeper understanding of the complex advection-dispersion-inactivation processes. In this report the construction and the solution of the equations of an analytical model that guided all the subsequent modelling activities is described. The **tracer** and the **bacteria** fields are obtained as products of a function of time and the horizontal coordinates by a series of decaying exponential functions of time weighted by functions of depth. The quotient between the bacteria concentration and the tracer concentration, that is commonly used to determine a global value of the T_{90}, taking suitable average values after a long enough transient, is studied. A procedure that may be used to summarize the field of local inactivation times by a few parameters, determined by **tracer experiments** and **microbiological measurements**, is discussed. A half-empirical correlation formula between the T_{90} parameter and the main variables of the body of receiving waters is suggested from the results of tracer experiments and other sources of information. The advantages and limitations of the modelling approach used in this case are assessed and some possible improvements are briefly outlined.

Key-words: mathematical models, tracers, bacterial inactivation time, sewage, estuarine coastal waters

(A) Introduction:

When sewage is discharged in the coastal waters of a river, an estuary or the sea, the bacterial concentration decreases due both to physical dilution and to death by adverse conditions in the body of receiving waters. The killing rate of micro-organisms due to the body of receiving waters depends of temperature, salinity and ultraviolet radiation, amongst other environmental parameters, such as other pollutants, nutrients and possible predators.

The inactivation or death is expressed as a T_{90} value, which is the time it takes for bacterial concentration to decrease by a factor of 10 beyond the decrease due to dilution. As the nature of this process of self-purification is not completely known, it is in general not possible to predict the value of T_{90} from the properties of the receiving water, albeit there are some half-empirical correlations that may be used to obtain preliminary estimations. So, an experimental determination of T_{90} must be done, as a rule.

To do this, a **population of micro-organisms** is injected in the site and its concentration is measured at different instants and in different positions in the body of receiving waters.

To distinguish the effect due to advection and dispersion of the population, from the killing effects of the environmental factors, a **tracer** is usually used. The tracer is injected jointly with the population of micro-organisms, and its concentrations are measured at the same instants and positions. Then, if the tracer behaves as a **conservative pollutant**, and if it is transported in the same way as the bacterial population, its dilution must be due only to transport processes. If we use a radioactive tracer with a half-life short enough to be taken into account, it is always possible to make a correction for tracer disintegration and after doing that, continue as it were a conservative tracer. In this case the time evolution of the quotient between the concentration of still alive bacteria and the tracer concentration (corrected for disintegration if necessary) measured at the same instants and at the same positions, would give us a measure of the capacity for self-purification of the receiving waters. With this information, together with information about currents and other data, that are needed as inputs to be introduced in suitable mathematical models, it is possible to calculate, as outputs of these models, what would be the micro-organism concentrations in certain critical points (near shorelines, for example) given a location, length, discharge flow, and so on, of an intended outfall discharge of sewage waters.

In estuaries like Río de la Plata, it is fairly common, mainly during summer, early autumn and late spring time, to find a strong vertical stratification. The salinity (and density) increases significantly from the free surface to the bottom, and often two or three layers of different densities and salinities can be observed.

Temperature differences between surface and bottom exist, but are usually less significant.

A variable charge of suspended sediments blocks the ultraviolet rays, whose killing effect is thus produced mainly in a layer of water adjacent to the free surface, and much less or not at all in grater depths, near the bottom.

As a consequence of all these variations, the kinetics of bacterial death is a fairly complex and depth dependent process. So, it is reasonable to ask about the meaning of the experimental results obtained during the above mentioned experiments intended to quantify the self-purifying capacity of estuarine waters. We will discuss this meaning using a fairly simple mathematical model of the processes of advection, dispersion and inactivation.

(B) A simple transport model with decay terms dependent of depth:

We start from the following field equation for the concentration $c(t,x,y,z)$ of a non conservative pollutant: $\frac{\partial c}{\partial t} = \hat{L}_h[c] + \hat{L}_v[c] - K(z).c$ [1]

The operator $\hat{L}_h$ describes the horizontal advection and turbulent diffusion, while the operator $\hat{L}_v$ describes the vertical turbulent diffusion, and if it is significant, the sedimentation process. Both operators, applied to the concentration field, are linear.
The hydrodynamics related with the advection processes is assumed to be given.
At this level of description the horizontal eddy diffusivities may be scale dependent.
However we suppose that the field of local inactivation rates $K(z)$ depends only of the vertical coordinate z. (The z axis points upwards from the bottom towards the surface of free water). This dependence allows us to take into account the vertical salinity gradients, the varying effects of ultraviolet light due to the absorption processes, and so on.
If $E_v(z)$ is the vertical eddy diffusivity and w_s is the sedimentation velocity, we can pose the following boundary conditions (Nihoul, 1975, chapter1):
At the surface: $-E_v \frac{\partial c}{\partial z} - w_s c = 0$ [2a]. At the bottom: $-E_v \frac{\partial c}{\partial z} - w_s c = -w_s c.\left(1 - \frac{\tau_b}{\tau_c}\right)$ [2b]
In [2b], τ_b is the shear stress at the bottom, while τ_c is a critical value of τ_b such that above it the erosion rate is greater than the deposition rate. This is only an approximate boundary condition (Fredsoe and Deigaard, 1992) but it suffices for our purpose.
Now let us consider a layer of the receiving water body of depth H (in our case less than 10 meters) and several hundred meters of horizontal extension l. Even if the vertical eddy diffusion coefficient E_v is one or two orders of magnitude less than the horizontal eddy diffusivities E_h, the vertical time scale of diffusion $t_v = H^2 / E_v$ is at least an order of magnitude less than the horizontal time scale of diffusion $t_h = l^2 / E_h$ and the time scale of sedimentation $t_s = \frac{H}{w_s}$. We may further assume that t_h is at least an order of magnitude less than the time scales of the tidal currents and the diurnal variations in the light intensity that reaches the surface of the water body.
Although the horizontal operator may show an explicit dependence of time and horizontal coordinates, (due to the advection terms and the scale effect on the horizontal eddy diffusivities), the operator $\hat{L}_v$ and the inactivation constant K may be considered as independent of time when trying to solve Equation [1].
Furthermore, to construct a simple mathematical model, we suppose that $\hat{L}_v$ is independent of the horizontal coordinates.

Then, substituting the **ansatz** $c(t,x,y,z)=\psi(t,x,y).Z(z)$ in this equation and introducing a separation of variables constant k^2 we obtain:

$$-\hat{L}_v[Z]+K(z)Z=k^2.Z \qquad [3] \qquad\qquad \frac{\partial\psi}{\partial t}=\hat{L}_h[\psi]-k^2.\psi \qquad [4]$$

Introducing the auxiliary field $\psi_0(t,x,y)=e^{k^2t}\psi(t,x,y)$, it verifies the horizontal advection-diffusion equation like an already vertically well mixed and conservative pollutant or tracer: $\frac{\partial\psi_0}{\partial t}=\hat{L}_h[\psi_0]$ Meanwhile ψ is given by: $\psi=\psi_0.e^{-k^2t}$

The vertical operator is given by $L_v[c]=-\frac{\partial}{\partial z}\left(E_z(z)\frac{\partial}{\partial z}c\right)-w_s\frac{\partial c}{\partial z}$ so equation [3] may be written:

$$-\frac{d}{dz}\left(E_v(z)\frac{d}{dz}Z(z)\right)-w_s\frac{dZ(z)}{dz}+K(z).Z(z)=k^2Z(z) \qquad [5]$$

If $w_s=0$, the differential operator is already in self-adjoint form.

In any case, it can be put into a self-adjoint form multiplying the equation by the function:

$$\rho(z)=\exp\left(+w_s\int_0^z\frac{dz'}{E_v(z')}\right) \qquad [6]$$

From the boundary conditions [2a], [2b] applied to the **ansatz,** we have, if $z=0$ represents the bottom and $z=H$ the surface of the water body:

$$-E_v(0)\frac{dZ(0)}{dz}-w_sZ(0)=-w_sZ(0).\left(1-\frac{\tau_b}{\tau_c}\right) \quad [7a] \qquad\qquad -E_v(H)\frac{dZ(H)}{dz}-w_sZ(H)=0 \quad [7b]$$

From equation [5] in self-adjoint form, jointly with the homogeneous boundary conditions [7], we have an eigenfunction ($Z(z)$)-eigenvalue (k^2) problem of the Sturm-Liouville type. If $E_v(z)$ is positive and $K(z)$ non-negative, and both functions are regular enough, there is a denumerable set of eigenvalues $k_n{}^2$: $0\le k_0{}^2< k_1{}^2< k_2{}^2<\ldots< k_n{}^2<\ldots$ There is a single eigenfunction $Z_n(z)$ corresponding to each eigenvalue $k_n{}^2$, and the eigenfunctions corresponding to different eigenvalues are orthogonal relative to the weigth $\rho(z)$:

$$\int_0^H\rho(z)Z_p(z).Z_q(z).dz=0 \qquad p\neq q$$

(From now on we consider normalized eigenfunctions: $\int_0^H\rho(z)(Z_p(z))^2dz=1$).

The initial condition for the concentration field depends of how the injection of the pollutant or tracer is made.

Usually it is possible to pose:

$$c(0;x,y,z)=M_o.\delta(x).\delta(y).f(z) \qquad [8]$$

Here M_0 is the total mass of tracer or pollutant **suddenly** injected, while $\delta(x)$ and $\delta(y)$ are Dirac's distributions along the horizontal directions. They stem from the assumption that the horizontal size of the mass of tracer or pollutant, immediately after the injection, is negligible in comparison with the horizontal scales of transport by advection and turbulent diffusion.

The function $f(z)$ reflects the vertical distribution of the injected tracer or pollutant immediately after the injection. It verifies $\int_{z_i}^H f(z).dz=1$. Here z_i gives the vertical coordinate of the deepest point of the injection, so $H-z_i$ is the depth of injection measured from the surface.

However, for an asymptotic analysis of the process, it is possible to neglect the details of the vertical distribution of the injection.

The solution of [1] with boundary conditions [2] and initial condition [8] can be represented as:
$$c(t,x,y,z)=\sum_{n=0}^{\infty}e^{-k_n{}^2t}\psi_n(t;x,y).Z_n(z) \qquad [9]$$

Then:
$$c(0,x,y,z)=\sum_{n=0}^{\infty}\psi_n(0;x,y).Z_n(z)$$

From [7] it follows:
$$\psi_n(0;x,y)=M_0.\left(\int_0^H\rho(z)f(z)Z_n(z).dz\right)..\delta(x).\delta(y) \qquad [10]$$

This is the initial condition that we must use jointly with [4] to find $\psi_n(t;x,y)$.

These functions are solutions of the same advection-diffusive transport equation (Equation [4]) jointly with the same boundary conditions for each of them.

The only difference appears in the initial condition for each n, given by [10].

So, if $\psi_0(t;x,y)$ is the solution of [4] with the same boundary conditions (not yet specified) but with the initial condition $\psi_0(0;x,y)=\delta(x).\delta(y)$, we have:

$$\psi_n(t;x,y)=M_0.f_n.\psi_0(t;x,y) \qquad [11a] \qquad\qquad f_n=\int_0^H\rho(z)f(z).Z_n(z).dz \qquad [11b]$$

The only difference between the different functions ψ_n appears in a proportionality factor, but the space-time dependence, as given by $\psi_0(t;x,y)$, should be the same for all of them. As a consequence, [8] may be written thus:
$$c(t;x,y,z)=M_0.g(t,z).\psi_0(t;x,y) \qquad [12]$$

Here, by definition,
$$g(t,z)=\sum_{n=0}^{\infty}e^{-k_n{}^2.t}f_n.Z_n(z) \qquad [13]$$

From [12] we can calculate the concentration field of the pollutant (or tracer) for $t\geq 0$ and for each point of the body of estuarine waters that we are studying.

So, assuming that we can determine $k_n{}^2$ and $Z_n(z)$, the only task that remains is to give a concrete solution $\psi_0(t;x,y)$ for the horizontal transport. But **as we are going to consider the quotient between the concentration field $c_b(t;x,y,z)$ of a non-conservative pollutant and the concentration field for the tracer (considered as conservative) $c_T(t;x,y,z)$, it is not necessary to derive a formula for $\psi_0(t;x,y)$.**

The reason is that $\psi_0(t;x,y)$ **must be the same for both, pollutant and tracer**.

The components of the advection field are the same, the turbulent diffusion coefficients are the same, the boundary conditions for $\psi_0(t;x,y)$ are the same and the initial conditions for $\psi_0(t;x,y)$ are the same, so the field $\psi_0(t;x,y)$ must be the same for both of them.

(C) Calculation of eigenvalues and eigenfunctions by a regular perturbation approach

Let us consider now the eigenvalues $k_n{}^2$ and their corresponding eigenfunctions $Z_n(z)$. From equations [5], [6] and [7], following a standard procedure we derive the relation:
$$k_n{}^2=\int_0^H\rho(z).\left(E_v(z)\left(\frac{dZ_n(z)}{dz}\right)^2+K(z).Z_n{}^2(z)\right).dz+w_s.\left(-\frac{\tau_b}{\tau_c}.Z_n{}^2(0)+\rho(H).Z_n{}^2(H)\right) \qquad [14]$$

It is possible to obtain fairly good approximations to the kinetic coefficients substituting the exact eigenfunctions by approximate ones, derived by regular perturbation theory. The vertical sedimentation-diffusion equation can be written in self-adjoint form:

$-\hat{L}_v[Z]+\rho.K.Z=k^2.\rho.Z$ [15] , $\hat{L}_v[Z]=\frac{d}{dz}\left[\rho.E_v.\frac{dZ}{dz}\right]$ with ρ given by [6].

Let us introduce the averages over depth: $K_0=\frac{1}{H}\int_0^H K(z).dz$ [16] $E_0=\frac{1}{H}\int_0^H E_v(z).dz$ [17]

If we substitute, in equation [5], $K(z)$ and $E_v(z)$ by their average values, it is fairly easy to obtain a closed form solution for the eigenfunctions and the eigenvalues.

When diffusion time $t_v={H^2}/{E_0}$ is less than one third of the sedimentation time $t_s=\frac{H}{w_s}$, the **eigenfunctions** are given by:

$$Z_{0,n}(z)=\sqrt{\frac{2}{H}}.C_n.e^{-\frac{t_v}{2t_s}.\frac{z}{H}}.\cos\left(\frac{\omega_n.z}{H}-\theta_n\right)\quad n=0,1,2,3,...\qquad [18]$$

Here C_n is of the order of 1, ω_n is close to $n\pi$ and θ_n is close to zero.

The **eigenvalues** may be approximated by: $k_n{}^2\approx K_0+\frac{2}{t_s}.\left(1-\frac{\tau_b}{\tau_c}\right)+\frac{n^2.\pi^2}{t_v}$ [19]

In order to derive an improved approximation, we make the assumption:

$$K(z)=K_0+\varepsilon.K_1(z)\quad [20]\qquad E_v(z)=E_0+\varepsilon.E_1(z)\quad [21]$$

Here E_0 and K_0 are the average values given by [16] and [17], the parameter ε is a small number and the functions $K_1(z)$ and $E_1(z)$ are of the order of unity.

Then the vertical sedimentation-diffusion operator, $\hat{L}_v$, can be split thus:

$$\hat{L}_v=\hat{L}_0+\varepsilon.\hat{L}_1\qquad [22]$$

Then we split $k^2=k_0{}^2+\varepsilon.k_1{}^2$ [23] and $Z(z)=Z_0(z)+\varepsilon.Z_1(z)$ [24], where Z_0 and $k_0{}^2$ are given by [18] and [19] if sedimentation is slow enough.

Equation [15] can be approximated, up to the first order in ε, by these two equations:

$$\hat{A}[Z_0]=0\quad [25]\qquad \hat{A}[Z_1]=g_1(z)\quad [26]$$

By definition: $\hat{A}[Z_0]=-\hat{L}_0[Z_0]+\rho.K_0.Z_0-k_0{}^2.\rho.Z_0=0$ $\hat{A}[Z_1]=-\hat{L}_0[Z_1]+\rho.K_0.Z_1-k_0{}^2.\rho.Z_1$

$g_1(z)=\hat{L}_1[Z_0]-\rho.K_1.Z_0+\rho.k_1{}^2.Z_0$

The solution of [25] is known, as well as $k_0{}^2$. From the theorem of alternatives (Bender and Orzag, 1999) we obtain an equation for $k_1{}^2$, so that $g_1(z)$ is fully determined.

Then we can solve [26] in order to derive an expression for Z_1.

Substituting $Z_n(z)=Z_{0,n}(z)+\varepsilon.Z_{1,n}(z)$ in [14] we can get a better analytical estimation of $k_n{}^2$.

(D) Discussion and conclusions

From [12],the quotient of the concentrations of bacteria c_b and tracer c_T does not depend of the horizontal position (x,y), whenever both concentrations are taken in the same instant and in the same point, because $\psi_0(t;x,y)$ is the same for both and disappears. When the advection-dispersion process has advanced enough, the populations of bacteria and tracer are highly diluted. Then the quantities obtained taking local samples at a certain depth and at a certain horizontal position may be too scarce to enable good measurement results. So, let us suppose that we take samples in vertical columns, from

$z = H$ (the surface of free water) to $z = H - h$ (being h the length of a vertical sample taken with a suitable sampling tube).

From [12] it follows that:
$$\int_{H-h}^{H} c(t;x,y,z).dz = M_0.(\int_{H-h}^{H} g(t;z).dz).\psi_0(t;x,y) \qquad [26]$$

From [13] we obtain:
$$\int_{H-h}^{H} g(t,z).dz = \sum_{n=0}^{\infty} e^{-k_n{}^2.t}.f_n.\int_{H-h}^{H} Z_n(z).dz \qquad [28]$$

Forming the quotient of the integrals of the concentrations of bacteria c_b and tracer c_T taken along the vertical coordinate between $z = H - h$ and $z = H$ we obtain this new and better relation to apply in practice:

$$\frac{\int_{H-h}^{H} c_b(t;x,y,z).dz}{\int_{H-h}^{H} c_T(t;x,y,z).dz} = \frac{M_{0,b}.\int_{H-h}^{H} g_b(t,z).dz}{M_{0,T}.\int_{H-h}^{H} g_T(t,z).dz} = \frac{M_{0,b}}{M_{0,T}}(\frac{\sum_{n=0}^{\infty} e^{-k_{b,n}{}^2.t}.A_{b,n}}{\sum_{n=0}^{\infty} e^{-k_{T,n}{}^2.t}.A_{T,n}}) \qquad [29]$$

Here $A_{b,n} = f_{b,n}.\int_{H-h}^{H} Z_{b,n}(z).dz$ and $A_{T,n} = f_{T,n}.\int_{H-h}^{H} Z_{T,n}(z).dz$ are parameters that differ between bacteria and tracer, because not only the eigenvalues, but also the eigenfunctions may be different when one population (bacteria) suffers advection, dispersion, perhaps sedimentation, and inactivation, meanwhile the other population (conservative tracer) suffers advection and dispersion only.

From [29] and taking into account that for a conservative tracer $k^2{}_{T,0} = 0$, asymptotically when $t \to \infty$ it follows that:

$$\log_e\left(\frac{\int_{H-h}^{H} c_b(t;x,y,z).dz}{\int_{H-h}^{H} c_T(t;x,y,z).dz}\right) \approx -k^2{}_{b,0}.t + \log_e(\frac{M_{o,b}}{M_{0,T}}.\frac{A_{b,o}}{A_{b,T}}) \qquad [30]$$

In this relation, if we neglect sedimentation, $k^2{}_{b,0} = K_0 = \frac{1}{H}\int_0^H K(z).dz$ is inversely proportional to the parameter T_{90} measured in field experiments with bacteria and tracers. It is an average over depth of the field of local kinetic parameters $K(z)$.

If sedimentation is significant:
$$k^2{}_{b,0} = \frac{1}{H}\int_0^H K(z).dz + \frac{2}{t_s}.\left(1 - \frac{\tau_b}{\tau_c}\right)$$

In absence of transport processes the local concentration would decay according to an exponential law after a long enough time interval.

In general, taking into account possible variations from one point to another one, there is a whole field of decaying constants, a field of local values of T_{90} that would determine the local capacity for self-purification of the estuarine waters if the combined advection-dispersion process were negligible.

But as this combined process is not negligible, the description of the capacity for self-purification must be done by means of the double set of parameters $k_{b,n}$, $k_{T,n}$, $A_{b,n}$ and $A_{T,n}$ for $n = 0,1,2,3,...$ A denumerable set of parameters describe the self-purification process.

In practice a small number may be used to represent the experimental data after the initial stages of the process: $k^2{}_{b,0}, k^2{}_{b,1}, k^2{}_{T,1}, A_{b,0}/A_{T,0}$, $A_{b,1}/A_{T,0}$ and $A_{T,1}/A_{T,0}$, applying well known methods for parameter identification (Thyn and Zitny,2000) .

From previous work and experimental results, the following half empirical formula for a coarse (and generally conservative) estimation of T_{90} in hours was proposed:

$$\frac{1}{T_{90}} \approx K_0.e^{\frac{T_a - T_{a,1}}{T_{a,2}}}.e^{\frac{s}{s_0}} + \frac{2\alpha}{\pi}\left(1-(0.65)C^2\right)\left(1-\frac{S}{S_0}\right)$$

T_a: water temperature in ºC, s: salinity in $^{o}/_{oo}$; α: angle of the sun's direction to the horizontal plane, in radians; C: fraction of sky covered by clouds; S: solids in suspension, in $^{mg}/_{l}$; $K_0 \cong 0.023 h^{-1}$, $T_{a,1} = 20^o C$, $T_{a,2} = 52^o C$, $s_0 = 120\,^{o}/_{oo}$, $S_0 = 800\,^{mg}/_{l}$.

It can be used in a gross estimation of the duration of the field experiments in a given scenario or as an input to take into account the bacterial die-off in numerical computations using hydrodynamic models.

The following half empirical formula for $K_b(z)$ in the simplified analytical model of the stratified water body may be of some interest: $\frac{1}{T_{90}(z)} \cong \frac{K_b(z)}{2.3} \cong K_0.e^{\frac{T_a - T_{a,1}}{T_{a,2}}}.e^{\frac{s(z)}{s_0}} + K_1.I_0.e^{-c.(H-z)}$

being $c \cong \frac{\beta}{\sqrt{1-(1.33)^2.\cos^2\alpha}}$, β an average extinction constant in the water body, $s(z)$ the vertical salinity profile and α is the angle between the Sun direction and the horizontal plane as defined before.

Neglecting sedimentation: $k_0{}^2 = K_{0,b} = \frac{\int_0^H K_b(z).dz}{H} \cong \frac{2.3}{T_{90}}$. From the formula for $T_{90}(z)$

we obtain: $$\frac{1}{T_{90}} \cong \frac{K_{0,b}}{2.3} \cong K_0.e^{\frac{T_a - T_{a,1}}{T_{a,2}}}.(\frac{1}{H}\int_0^H e^{\frac{s(z)}{s_0}}.dz) + \frac{K_1.I_0}{c.H}\left(1-e^{-c.H}\right)$$

Appendix: A simple and naïf approach to bacteria die-off through T_{90}

If we could follow the trajectory of a mass of bacteria $c_b(t) = \frac{c_b(0)}{D(t)}.e^{-K_b.t}$ (Phelps (1944) formula for rivers) or equivalently $c_b(t) = \frac{c_b(0)}{D(t)}.10^{-\frac{t}{T_{90}}}$

Concentration of bacteria population $c_b(t)$; $D(t)$ dilution factor at time t; K_b die-off parameter; $T_{90} \cong \frac{2.3}{K_b}$

A conservative tracer of concentration $c_T(t)$ following the same trajectory would allow to measure dilution: $c_T(t) = \frac{c_T(0)}{D(t)}$ Then $\log_e \frac{c_b(t)}{c_T(t)} \approx -K_b.t + \log_e \frac{c_b(0)}{c_T(0)}$ would allow us to determine the die-off constant K_b.

In a homogeneous body of water, homogeneous both from the advection-dispersion and from the bacterial inactivation point of view, this simple approach can be applied.

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